Effect of Silicon Incorporation in Iron: Equation of State and Phase Transition

J. Zhang (CHiPR, SUNY, Stony Brook) and F. Guyot (U. of Paris)

Experiments have been carried out on iron and two iron-silicon alloys, $Fe_{0.91}Si_{0.09}$ and $Fe_{0.83}Si_{0.17}$, at high pressure and temperature up to 9 GPa and 1473 K, using a DIA-type, cubic-anvil, high-pressure apparatus interfaced with synchrotron X-ray diffraction. Pressure-volume-temperature data were obtained for iron and $Fe_{0.91}Si_{0.09}$ and are analyzed using Birch-Murnaghan equation of state. With fixed K_0 at 4, we obtain for iron:

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$$K_0 = 154(2)GPa$$

$$(\delta K/\delta T)_P = -0.041(5)GPaK^{-1}$$

and

$$\alpha_{300-773} = 4.46(12)K^{-1};$$

for $Fe_{0.91}Si_{0.09}$, we have

$$K_0 = 156(2)GPa$$

$$(\delta K/\delta T)_P = -0.044(6)GPaK^{-1}$$

and

$$\alpha_{300-773} = 4.71(14)K^{-1}$$
.

These results indicate that substitution of small amount of Si in iron would not have a significant effect on the equation of state parameters. Phase transition were studied in two experiments, one with iron and $F_{0.91}Si_{0.09}$ loaded in the boron nitride container and the other $Fe_{0.91}Si_{0.09}$ and $Fe_{0.83}Si_{0.17}$. The bcc-fcc phase transition in $Fe_{0.91}Si_{0.09}$ was observed at 7.5 and 9 GPa, but the temperatures of transition are more than 300 K higher than those in iron. Phase transition was not observed at 5 GPa and lower pressures in $Fe_{0.91}Si_{0.09}$ and in the entire experimental pressure and temperature range for $Fe_{0.83}Si_{0.17}$. These observations indicate that incorporation of Si in iron strongly stabilizes the bcc structure in the system Fe-Si. In comparison with literature data at 1 atm., the present results also provide constraints on the compositional maxima of the γ -loop for the system Fe-Si as a function of pressure.